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A VERIFICATION AND VALIDATION PROCEDURE FOR COMPUTATIONAL FLUID DYNAMICS SOLUTIONS

by

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14. ABSTRACT

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Abstract

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Administrative Information

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Introduction

Computational fluid dynamics (CFD) solutions are increasingly being used as input for the engineering design process within the naval hydrodynamics community. Naval combatants in particular are going through revolutionary design changes for, among other things, improved stealth [Valenti, 2001]. The new combatant concepts are sufficiently different from traditional hull forms that existing databases and empirical formulas typically used for design are no longer applicable. This has required the evolution of a new paradigm for ship design that is more reliant than ever on CFD [Rood, 2000]. In the past Reynolds-averaged Navier-Stokes (RANS) numerical predictions have mainly been used to evaluate trends and differences between related geometries. However, the drive for more reliance on numerical predictions is creating a desire to obtain absolute values from these computations as well as a better understanding of their accuracy. This is motivating the development of methods for performing verification and validation (V&V) analyses [Roache, 1998] to assess the numerical and modeling uncertainty of these predictions.

The approach presented in this report is based on the work of Stern et al. [1999]. The interested reader should consult Stern et al. [1999] for details of the theory and meaning of the verification and validation process. This particular approach is just one of various approaches being put forth in the literature. Indeed, much interest has been paid to the topic of verification and validation in recent years. Verification and validation policies and guidelines have been developed by various organizations including AIAA [1998] and ASME [Freitas, 1993] along with numerous journal papers dedicated to the topic. Concurrently, there are efforts by the experimental community to provide benchmark data sets for V&V. Recent measurements taken for DTMB Model 5415 are an example of this effort [Ratcliffe, 2000]. Although there is no universally accepted V&V procedure, the V&V process is the beginning of a methodology to provide some information on the level of confidence in a computational solution and will most

likely become another important factor to be used by the community in evaluating a computational solution.

Procedure

The verification and validation procedure presented here involves making uncertainty estimates of numerical predictions at the location of experimental data points. Using the terminology of Stern et al. [1999], verification is defined as the process of assessing the numerical uncertainty (U_{SN}). Typically, the most significant sources of numerical uncertainty in a RANS calculation come from the use of finite grid sizes, finite time steps, and the use of iterative solution methods. The majority of this report focuses on the estimation of the uncertainty in the numerical prediction due to the influence of finite grid sizes. This uncertainty estimate requires that numerical solutions be obtained on more than one grid. Validation is defined as the process of assessing simulation modeling uncertainty. Simulation modeling uncertainty is caused by assumptions and approximations in the mathematical representation of the physical problem. As an example, one common source of simulation modeling uncertainty would be the use of a turbulence model. In this procedure assessing the simulation modeling uncertainty is accomplished by comparison with benchmark experimental data. Stern et al. [1999] defines a quantity called the validation uncertainty (U_V).

$$U_V^2 = U_D^2 + U_{SPD}^2 + U_{SN}^2$$

The terms on the right hand side of this equation are defined as follows.

U_D=Estimated experimental data uncertainty

U_{SPD}=Estimated simulation previous data uncertainty

U_{SN}=Estimated simulation numerical uncertainty

In this procedure these uncertainty estimates are made at the location of the experimental data points and the validation procedure is accomplished by determining if the difference between the numerical prediction and benchmark experimental data, known as the comparison error, is within the validation uncertainty at these locations. Thus, a numerical prediction is considered validated "at the U_V level" if,

$$|E| < U_V$$

where,

E = D-S = Comparison Error

D = Experimental data

S = Simulation result (i.e. numerical prediction)

This report assumes that the estimate of the uncertainty in the experimental data (U_D) has been provided by the experimentalists and that the estimate of simulation previous data

uncertainty (U_{SPD}) is known or is negligible. Simulation previous data uncertainty could come from such things as uncertainty in fluid properties or uncertainty in any experimental data used as input for the numerical simulation. This report will therefore focus on the simulation numerical uncertainty (U_{SN}). U_{SN} itself is a combination of other uncertainties of which the two most significant for steady state solutions, grid uncertainty (U_G) and iterative convergence uncertainty (U_I), are considered in this report.

$$U_{SN}^2 = U_G^2 + U_I^2$$

where,

U_G=Estimation of grid uncertainty

U_I=Estimation of iterative convergence uncertainty

It is recommended that whenever possible the numerical solution be run to a point where iterative convergence errors become negligible. It is recognized, however, that for complex problems this may not be possible for all variables, in all areas, of all grids. When iterative convergence uncertainty is on the finest grid it can simply be added to the total uncertainty as outlined in Stern et al. [1999]. When it occurs on the coarser grids the procedure is less clear and a value for the uncertainty of the calculation is less easily obtainable. When performing a V&V analysis on a large field of data, providing iterative convergence for all values can be unrealistic because of the huge number of data points involved. Consequently, it is recommended that the iterative histories of a representative sample of the quantities being verified be examined to assess iterative convergence. In the absence of a clear method for computing an iterative uncertainty which is known to be non-negligible, it is recommended that an effort be made to provide statements regarding where the iterative convergence uncertainty is significant and, hence, where the simulation numerical uncertainty estimates cannot be regarded as accurate.

The remainder of this section will be used to document the procedure recommended for estimating the grid uncertainty (U_G). The grid uncertainty is an estimate of the confidence level one has that the solution has achieved grid independence based on comparisons with solutions from coarser grids. Ideally at least three grids would be used: a fine, medium, and coarse grid. The numerical results to be validated are computed for all grids, including any integrated quantities, and any field data that is to be directly validated must be interpolated to the locations of the experimental data. Prior to estimating the grid uncertainty the numerical results from the related grids must be used to compute the convergence ratio from which the convergence condition is determined. The convergence condition must indicate that the solutions are converging in order for a grid uncertainty estimate to be made.

Determination of the Convergence Condition

For validating single point quantities, or integrated quantities that are associated with the entire data set (i.e. the drag of a body), the following definition for a quantity known as the convergence ratio (R) is used.

$$R = e_{21} / e_{32}$$

The quantities e_{21} and e_{32} are simply the differences in the medium and fine grid predictions and the coarse and medium grid predictions respectively (i.e. $e_{21}=S_2-S_1$ and $e_{32}=S_3-S_2$, where S_1, S_2 and S_3 are the predictions from the fine, medium and coarse grids respectively). For validating a set of field data (i.e. a boundary layer profile, surface wave height, surface pressure map, etc.) it is recommended that the L2 norm of e_{21} and e_{32} be computed over the range of data being considered to obtain a "global convergence ratio" as defined below.

$$\langle R \rangle = \|e_{21}\|_2 / \|e_{32}\|_2$$

where,

$$\|e_{21}\|_2 = \left[\sum_{i=1}^{N} (e_{21_i})^2 \right]^{1/2}$$

$$\|e_{32}\|_2 = \left[\sum_{i=1}^{N} (e_{32_i})^2 \right]^{1/2}$$

This "global convergence ratio" is recommended in order to avoid situations where a few ill conditioned points, within the profile or field data set, are prevented from undergoing the verification and validation process.

Based on the computed value of R or ⟨R⟩ the convergence condition is determined as outlined below.

- Integrated or single point quantities:
  - R<0: An oscillating condition is implied by these 3 particular solutions
  - R>1: A divergent condition is implied by these 3 particular solutions.
  - 0<R<1: A convergent condition is implied by these 3 particular solutions.
- Field and profile data:
  - ⟨R⟩>1: On average a non-convergent condition is implied by these 3 particular solutions.
  - 0<⟨R⟩<1: A convergent condition is implied by these 3 particular solutions.

If the convergence condition is determined to be divergent/non-convergent (R>1 or ⟨R⟩>1) no grid uncertainty estimate can be made using the procedure of Stern et al. [1999]. Also, if the convergent condition is determined to be oscillating (R<0) no grid uncertainty can be estimated without performing more numerical simulations. Refer to Stern et al. [1999] for further discussion on this topic. The next section describes the recommended methods for estimating the grid uncertainty for data with convergent convergence conditions (0<R<1 or 0<⟨R⟩<1).

Estimation of the Grid Uncertainty

In this report, estimation of the grid uncertainty is performed following one of two methods. The first estimate is based on the methodology of Stern et al. [1999] and at its core uses Richardson extrapolation. The following equations define this grid uncertainty estimate.

$$U_G = |Cd_{RE}| + |(1-C)d_{RE}|$$

where,

$$C = \left(r^p - 1\right) / \left(r^{pth} - 1\right)$$

$$d_{RE} = e_{21} / \left(r^p - 1\right)$$

$$p = \ln(1/R)/\ln(r)$$

r = grid refinement ratio

p_{th} = theoretical order of accuracy

e_{21}=S_2-S_1

R = convergence ratio

In these equations, C is referred to as the correction factor, p as the order of accuracy estimate, and d_{RE} as the Richardson extrapolation error. The convergence ratio and the grid refinement ratio are used to compute the order of accuracy estimate. Strictly speaking, the grid refinement ratio is defined as the ratio of grid spacing between two successive grids. For practical problems the grid refinement ratio is somewhat difficult to define due to the non-uniformity of the grids used in solving such problems. Studies found in the literature indicate that the use of global parameters, such as the overall number of grid points, to compute the grid refinement ratio can be used for geometrically similar grids that make appropriate consideration for the physics of the problem [Celik, 1997]. The equations given above are valid only when the grid refinement ratio is constant for all successive grids. The order of accuracy estimate is then used to compute the Richardson extrapolation error. The correction factor is used in an attempt to correct for poor order of accuracy estimates, which can occur when one or more of the solutions is not in the asymptotic range. Again, refer to Stern et al. [1999] for a detailed discussion of these equations and their origins. The next section illustrates the use of this grid uncertainty estimation method.

Example: Verification and Validation of a Wave Profile

The procedure outlined above is applied here to a predicted wave height profile obtained with the Reynolds Averaged Navier-Stokes (RANS) code UNCLE [Taylor, 1991] on three related grids. The coarse and medium grids were obtained by removing every other point from the next finer grid, giving a grid refinement ratio of 2.0. Figure 1 provides a comparison between the fine grid numerical prediction and the experimentally measured wave profile. The wave height profiles predicted by the three different grids are shown in Figure 2. For this example the L2 norms of e_{21} and e_{32} are computed over the range of data points that make up the wave profile to come up with a "global convergence ratio".

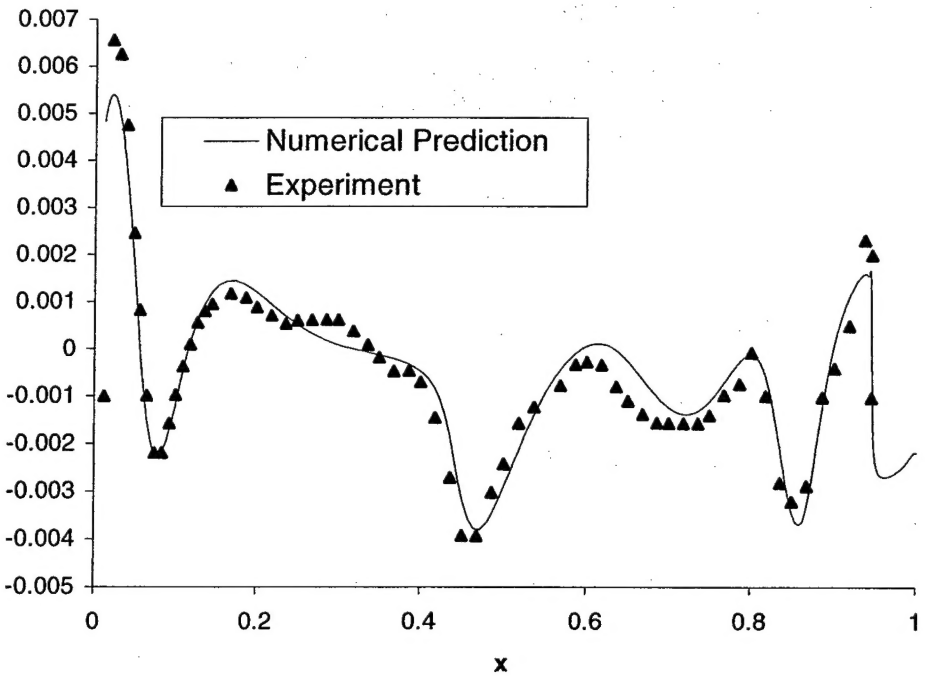

Fig. 1. Predicted wave height from fine grid solution and experimental data.

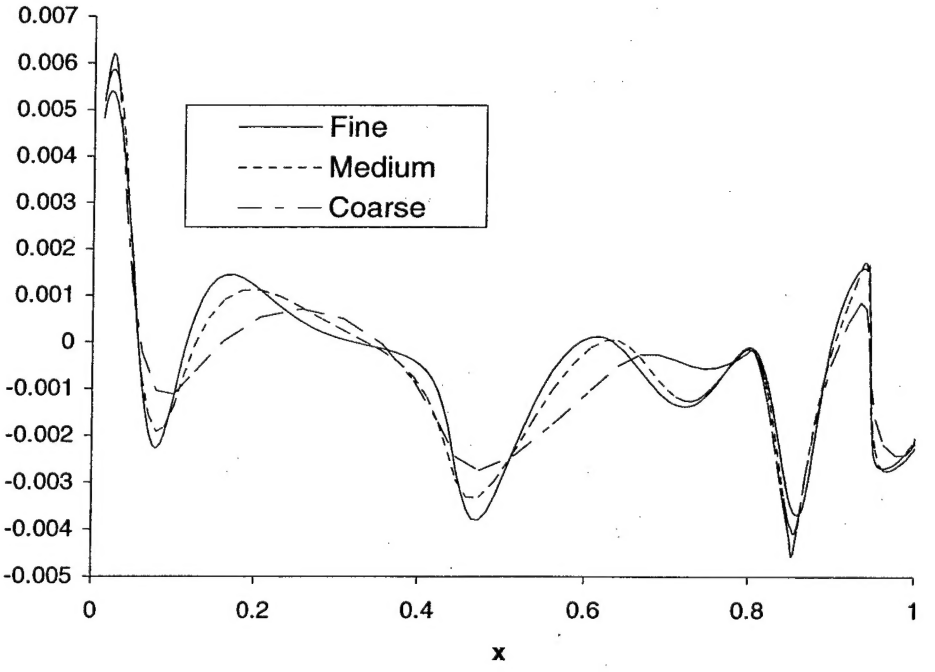

Fig. 2. Numerically predicted wave height on the hull for all three computational grids.

$$\|e_{21}\|_2 = \left[\sum_{i=1}^{N}(e_{21_i})^2\right]^{1/2} = .00276$$

$$\|e_{32}\|_2 = \left[\sum_{i=1}^{N}(e_{32_i})^2\right]^{1/2} = .00397$$

$$\langle R\rangle = \|e_{21}\|_2 / \|e_{32}\|_2 = 0.695$$

Based on this computation it is determined that a convergent condition is implied by these 3 particular solutions, hence the grid uncertainty can be estimated using the method outlined in the previous section. The UNCLE code uses a 3rd order upwind scheme for the convective terms and a 2nd order central difference scheme for the viscous terms. Realistically, because of grid stretching and other factors one would normally expect the order of accuracy of the scheme to be between 1st and 2nd order. Therefore, the theoretical estimate of the order of accuracy for this particular example is chosen to be 2. Applying this method produces the following results.

$$r = 2$$

$$p_{th} = 2$$

$$R = 0.695$$

$$p = 0.525$$

$$C = 0.146$$

From these numbers the grid uncertainty is estimated at all of the points which make up the interpolated fine grid wave profile using the equations (repeated below) given in the procedure.

$$U_G = |Cd_{RE}| + |(1-C)d_{RE}|$$

$$d_{RE} = e_{21}/\left(r^p - 1\right)$$

Note that even if a "global convergence ratio" is used, the quantity e_{21} in the equation for the Richardson extrapolation error is computed individually for each point. Figure 3 indicates the result of this computation by plotting the fine grid solution along with two lines that represent the estimated grid uncertainty band for that solution. The validation procedure is carried through using the estimated grid uncertainty and an experimental uncertainty of 7.72×10^{-4}, which was provided by the experimentalist. For this example the iterative convergence uncertainty (U_I) has been ignored. A comparison between the validation uncertainty and the absolute error between the computation and experiment is shown in Figure 4. It can be seen that for the most part the figure indicates a validated solution "at the U_V level."

This method for estimating the grid uncertainty requires three related grids and is founded on the assumption that these three grids produce solutions that are in the asymptotic range. This is a very difficult requirement for a highly complicated geometry. While evaluating the RANS computations obtained with UNCLE it became apparent that the coarsest grid produces solutions that are definitely outside of the asymptotic range, at least for the wave height example documented here. This can be inferred from the order of accuracy estimate, p, obtained from the

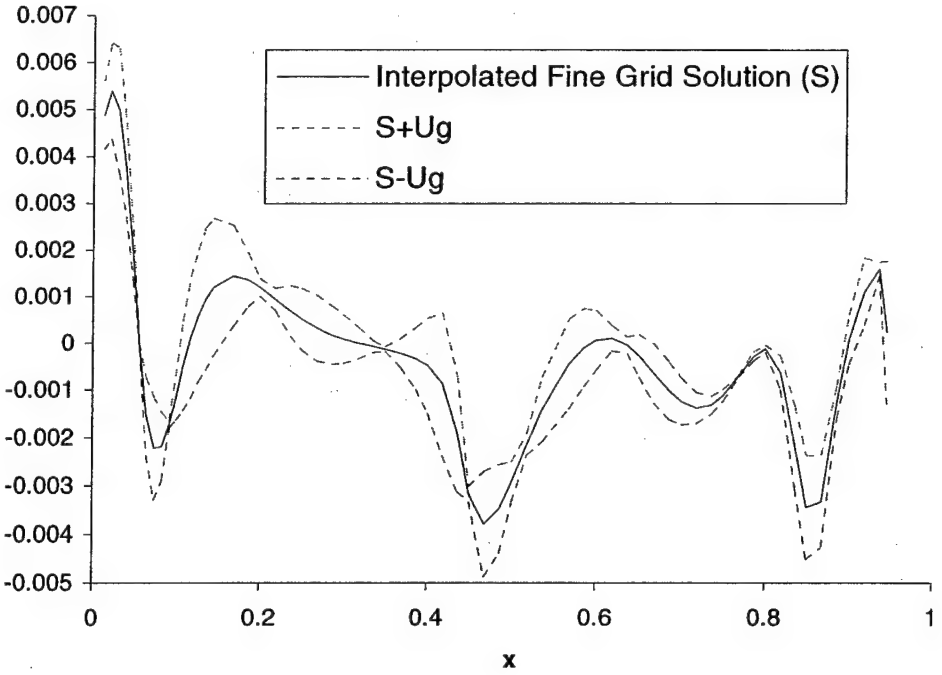

Fig. 3. Fine grid numerical prediction and the grid uncertainty band as estimated using the procedure of Stern et al. [1999].

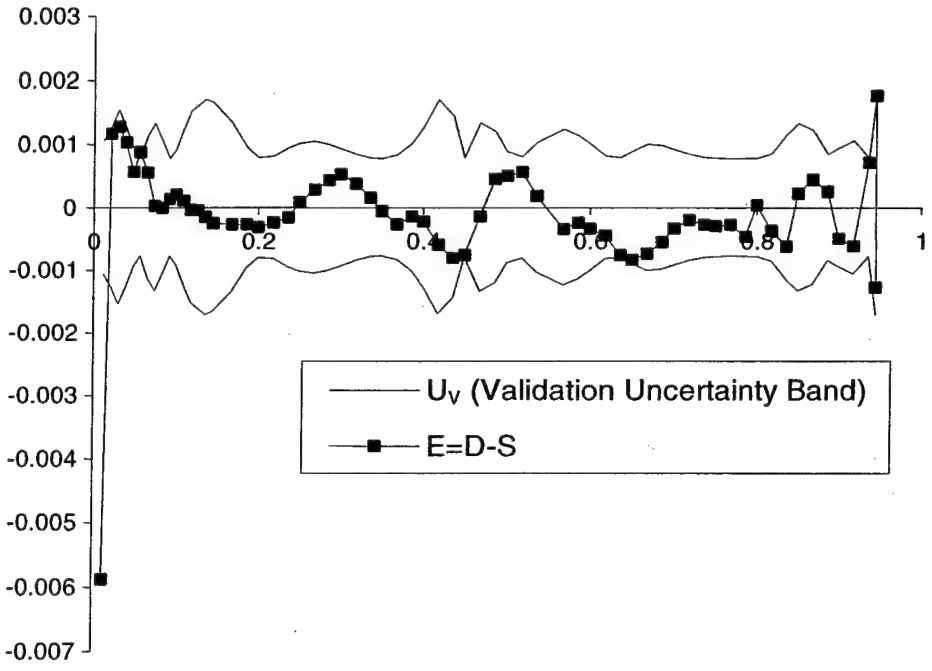

Fig. 4. Validation plot obtained with the grid uncertainty estimated using the procedure of Stern et al. [1999].

three solutions. As already discussed, one would normally expect the order of accuracy of the scheme to be between 1st and 2nd order. Although it is possible to get orders of accuracy somewhat less than theoretical, a value of 0.525 seems unrealistically low particularly for the medium and fine grids used here. On top of this, we know that the equation for p (p=ln(1/R)/ln(r)) is a poor estimate for the order of accuracy when all three grids are not in the asymptotic range. The correction factor, C, introduced by Stern et al. [1999] is an attempt to correct for values of p that are well outside of the expected theoretical range. This correction factor seems to have the correct type of effect for high values of p by making more conservative estimates on the numerical uncertainty. It can be seen from the equation for the estimated grid uncertainty that,

$$\text{If } p>>p_{th}\ (C>>1) \Rightarrow U_G \approx 2|Cd_{RE}|$$

However, for values of p that are less than the theoretical order of accuracy the nature of the equation for the estimated uncertainty is such that no correction at all is made.

$$\text{If } p \leq p_{th}\ (C \leq 1) \Rightarrow U_G = |d_{RE}|$$

This is the correct behavior for p sufficiently close to p_{th}. However, this can lead to overly conservative estimates for the uncertainty on the numerical solution when p is significantly below the theoretical value. This appears to be the case for this example, as seen from Figure 3. It can be argued that this method for estimating the grid uncertainty has produced an unfairly conservative estimate owing to the inclusion of solutions that are not in the asymptotic range.

Additionally, using the L2 approach for the estimate of R can give the impression a solution is not converging when it really is. The problem, again, is because the R computation is a measure of convergence based on all three grids. If the coarsest grid is outside the asymptotic range one can easily obtain a value of R that implies the solution is not converging, preventing an uncertainty estimate from being obtained with this approach. Consequently, it is recommended to use the approach of Stern et al. [1999] outlined above where it seems realistic. However, an alternative method is recommended in situations where the set of solutions do not meet all the criteria required for obtaining meaningful estimates of the grid uncertainty using the first method or when no estimate can be made at all. This alternative method is presented in the following section.

Alternative Estimation of Grid Uncertainty Based on 2 Grids

A recommended alternative estimate of the grid uncertainty is made based on an extrapolation using only the medium and the fine grid solutions. Although three grids are needed to demonstrate convergence, only two grids are needed to estimate sensitivity. Consequently it is felt that a better estimate of the uncertainty on the fine grid solution for this particular case would be to assume that the scheme is 1st order accurate and compute the uncertainty from the two finest grids. Again this estimate is still on the conservative side. This approach should be used when the estimate of p from the three grids is less than 1. It can, however, also be used when the computed p is significantly greater than 2. The basic assumption here is that the coarsest grid is an unrealistic prediction of the flow field and the medium and fine grids seem reasonable and consistent with each other. It is also assumed here that the fine and medium grids appear to be

converging to a particular solution. The equations for the uncertainty estimate reduce to the following equation.

$$U_G = e_{21} / \left(r^{p_{est}} - 1 \right)$$

where,

$p_{est} = 1$

r = grid refinement ratio

$e_{21} = S_2 - S_1$

This produces a grid uncertainty that is equivalent to the Grid Convergence Index of Roache [1998] for second order accurate solutions using the recommended "factor of safety" of 3.

Applying this approach to the predicted wave height, of the current example, results in the estimated grid uncertainty band shown in Figure 5 and corresponding validation comparison of Figure 6. The uncertainty band on the solution in Figure 5 is considerably smaller with this alternative method than that shown in Figure 3 even though the solutions on the fine and medium grids are exactly the same as before. This shows that the order of accuracy estimate, p, is driving the uncertainty bands. For the most part, both methods indicate a validated solution "at the U_V level," however, it is of interest to note that by using the less conservative estimate for the grid uncertainty, one actually obtains a more conservative estimate of U_V.

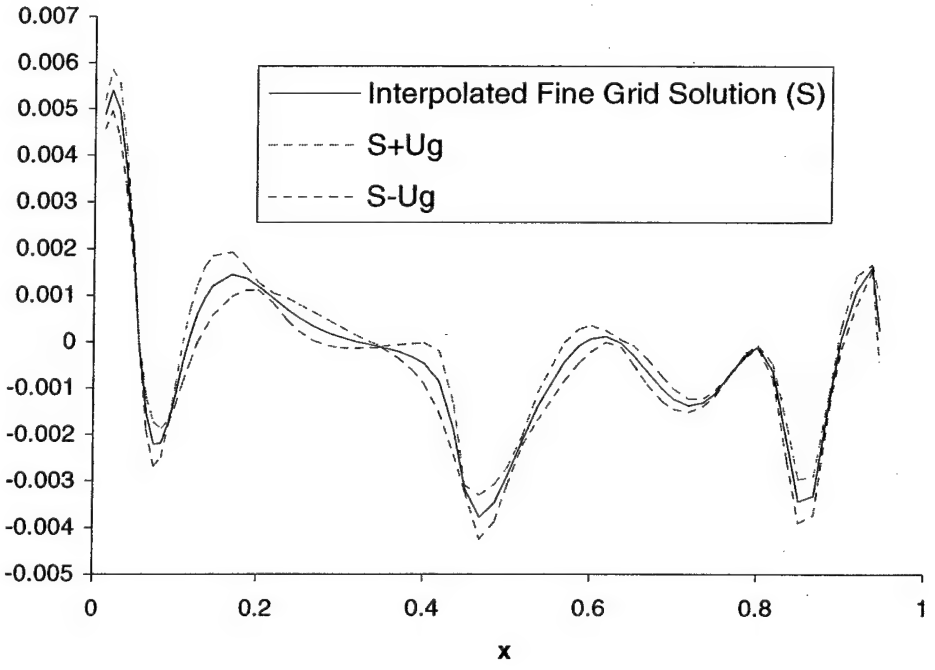

Fig. 5. Fine grid numerical prediction and the grid uncertainty band as estimated using the alternative procedure.

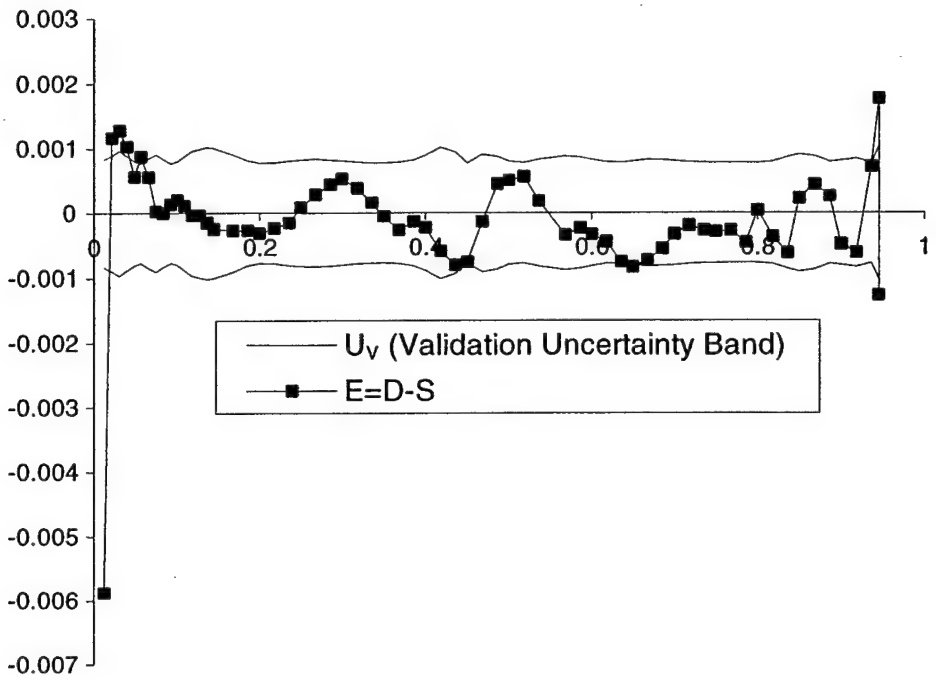

Fig. 6. Validation plot obtained with the grid uncertainty estimated using the alternative procedure.

Conclusions

This report has presented a procedure for performing a verification and validation analysis for computational fluid dynamic solutions. The procedure requires the estimation of uncertainties from many sources. In general it is advisable to eliminate, or render negligible, as much of the uncertainty as possible. In particular iterative convergence uncertainty is difficult to quantify and requires further study. In contrast, the estimation of the uncertainty due to the use of finite size grids has a relatively strong theoretical background. However, issues of a practical nature arise when making an estimation of the grid uncertainty for problems with complex geometry and physics. Problems occur when one or more of the solutions are not in the asymptotic range and the estimated order of accuracy is unrealistic. The approach of Stern et al. [1999] attempts to remedy this problem through the use of a correction factor. It has been shown in this report that the correction factor is appropriate in situations where the order of accuracy estimate is unrealistically high, but can lead to overly conservative estimates of uncertainty when the order of accuracy is estimated to be significantly below the theoretical value. An alternative method for estimating the grid uncertainty has been recommended for these situations, which requires solutions on only two grids and uses a conservative theoretical value for the order of accuracy.

Point-to-point comparison, as is done while validating field data following this procedure, can be problematic for data near inflection points where small changes in phase or position are not readily accounted for. Consequently, one should not loose sight of the traditional comparisons of experimental data and computations and base everything on the V&V results. It should be recognized that using numerical predictions at this level and using verification and validation methods of this type is really in its infancy and will most likely evolve over time.

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